UT-BATTELLE

Scientific Computing

Ricky A. Kendall
Group Leader, Scientific Computing
National Center for Computational Sciences

February 14th 2006

National Center for Computational Sciences

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

Outline

- Missions and Metric
- Staff
- Group Functions
  - Some of what we do

Missions and Metrics

- The Leadership Computing Facility
  - Delivery of breakthrough science in scientific areas critical to US DOE missions
- Scientific Computing Group
  - The mission of the Scientific Computing Group (SCG) is to facilitate, enable and accelerate breakthrough science through targeted collaborative efforts with users.
- Metrics for success
  - Delivery of breakthrough science!
    - Using the LCF resources provides insight and discovery.
  - Effective utilization of LCF resources.
  - User requirements effectively communicated to NCCS.
  - NCCS Enterprise Architecture expanded to meet user demands.
  - Applications ready for the next generation systems.

Path to accomplish our Mission

- SCG members serve as liaisons between project teams and the NCCS.
  - represent users in NCCS planning!!!
- We collaborate directly with NCCS project teams, augmenting and extending their computational and domain-specific expertise.
- Members of the SCG are research scientists with backgrounds in high performance computing, and various scientific domains.
- We directly help NCCS users realize increased scientific productivity through our extensive experience in porting, tuning, and developing software on NCCS resources.
- We reduce the total time to solution or insight for NCCS project teams by providing in-depth support for visualization, data movement and workflow needs, algorithmic development, and the choice and use of analysis tools.

Outline

- Missions and Metric
- Staff
- Group Functions
  - Some of what we do

The Staff

- Computational Science
  - Richard Barrett
  - Mark Fahey
  - Ricky Kendall
  - Jeff Kuehn
  - Bronson Messer
  - Richard Mills
  - Arnold Tharrington
  - Trey White
  - Vickie Lynch
- Visualization
  - Sean Ahern (Task Lead)
  - Ross Toedte
  - Jamison Daniel
  - George Ostrouchov
- End to End Solutions
  - Scott Klasky (Task Lead)














The Staff

- Computational Science
  - Richard Barrett
  - Mark Fahey
  - Ricky Kendall
  - Jeff Kuehn
  - Bronson Messer
  - Richard Mills
  - Arnold Tharrington
  - Trey White
  - Vickie Lynch
- Visualization
  - Sean Ahern (Task Lead)
  - Ross Toedte
  - Jamison Daniel
  - George Ostrouchov
- End to End Solutions
  - Scott Klasky (Task Lead)














The Staff

- Computational Science
  - Richard Barrett
  - Mark Fahey
  - Ricky Kendall
  - Jeff Kuehn
  - Bronson Messer
  - Richard Mills
  - Arnold Tharrington
  - Trey White
  - Vickie Lynch
- Visualization
  - Sean Ahern (Task Lead)
  - Ross Toedte
  - Jamison Daniel
  - George Ostrouchov
- End to End Solutions
  - Scott Klasky (Task Lead)
- New Hires (3)















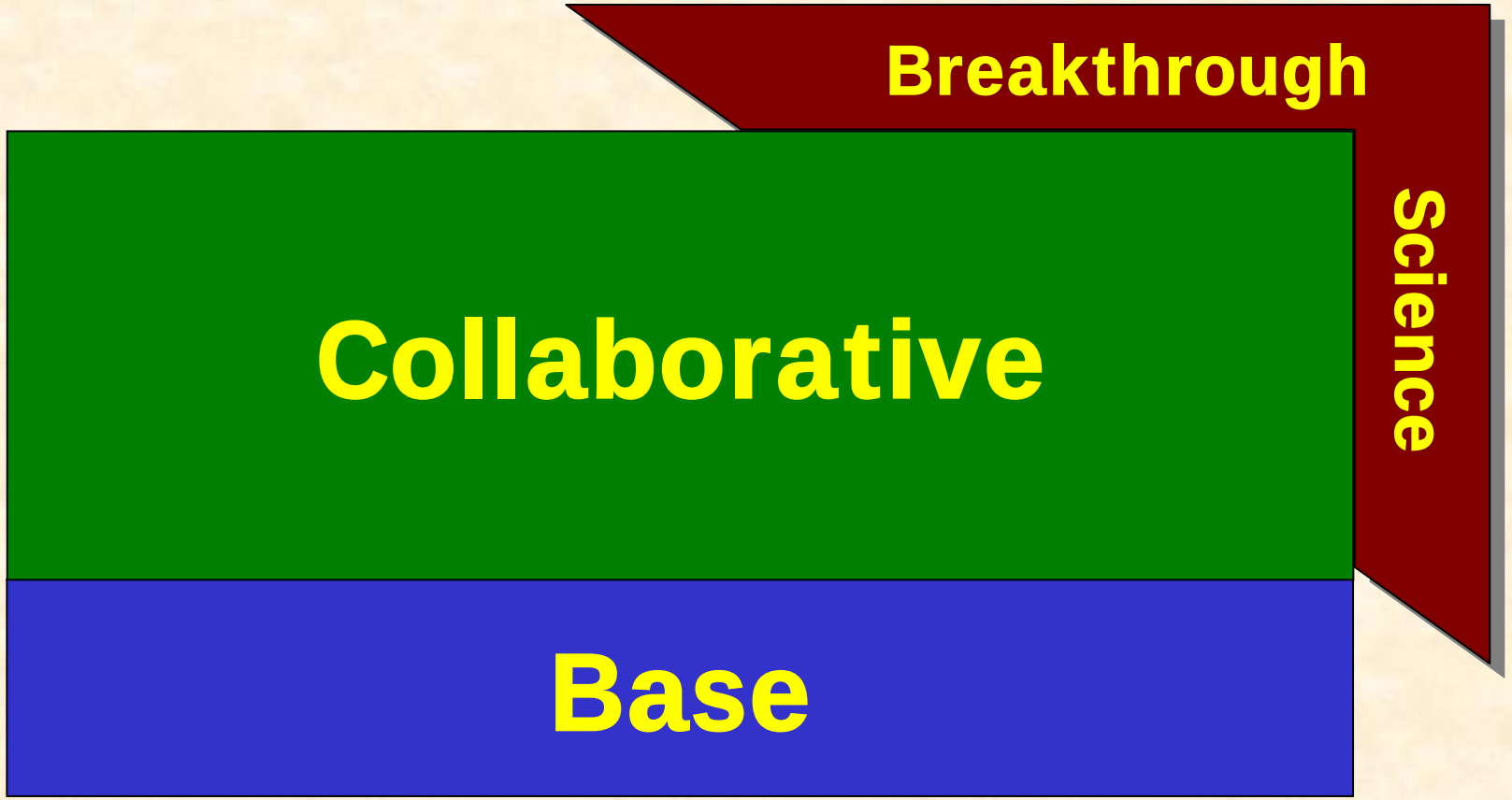


UT-BATTELLE

Outline

- Missions and Metric
- Staff
- Group Functions
  - Some of what we do

Scientific Computing Group Functions



Scientific Computing Group Functions

- Base functionality
  - Porting
  - Tuning
  - Development
- Collaborative
  - Algorithms
  - Applications
  - Libraries
  - Tools
  - Visualization
  - Workflow

Collaborative Functionality

- Synergism for leadership computing
  - With the NLCF Project Teams
    - Focusing the utilization of leadership resources
      - Computation, Data, Visualization, Productivity
    - Coordinating/Facilitating development of applications
      - Current and Future Needs
        - Today, Tomorrow, Where do you want to go!
  - With NCCS
    - Representing User requirements and expectations!
  - With Vendor Partners
    - Cray Center of Excellence

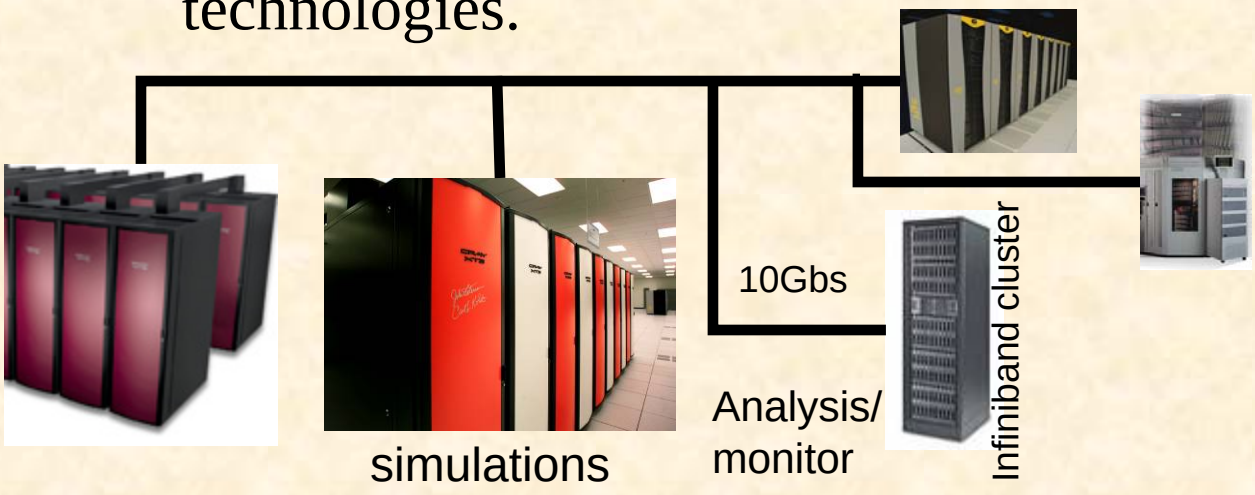
Scientific Computing Group Functions

Visualization within the NCCS

- Production Visualization Support
- Desktop Visualization Support
- Video Production
- Custom Application Support
- Visualization Facility
  - Operation and Support
- Research

End to End Solutions for the NLCF

- The principal mission of ORNL's “End-to-end” group is to aid researchers with tools to automate parts of the scientific investigation process.
  - Form a computational pipeline between the simulation and runtime-monitors/data analysis system.
  - Use a scientific workflow automation package to automate this process.
  - Allow users to concentrate on their “science” and not the technologies.




Questions?